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Components for computer-assisted structure elucidation

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Computer-Assisted Structure Elucidation (CASE) is of relevance for various fields in chemistry and biology such as natural products discovery or metabolomics. Here we report on several software components developed in our team over time which can form part of an integrated CASE package. We aim to design a user-friendly and flexible, yet powerful tool with Bioclipse [1] as the frontend. Bioclipse is an integrated software suite for chemo- and bioinformatics providing plug-ins for file handling and visualisation of compounds and spectra. Spectrum look-up and prediction is provided by our open NMR database NMRShiftDB [2], offering both 13C and 1H NMR prediction. We have recently demonstrated the prediction of proton NMR spectra based on NMRShiftDB data with an average error of 0.18 ppm [3]. The resulting CASE system will provide a choice of different structure generators, including stochastic search engines, based on Simulated Annealing and Genetic Algorithms.

References

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